Thermodynamic and Structural Properties of Water at the Interfaces with Inorganic Layered Materials: Molecular Dynamics Simulation

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Molecular-level understanding of thermodynamic, structural, and transport properties of aqueous species at the interfaces with inorganic materials and in their nano-pores is the key to understanding and predicting their functionality as adsorbents, ion exchangers, membranes, and in other technological applications. By performing molecular dynamics (MD) computer simulations, we were able to study complex structural environments and dynamical behavior of water molecules and a variety of cations and anions on and near the surfaces of several model inorganic layered materials, such as clays, layered double hydroxides, and hydrous cement phases. The structure and atomic composition of the substrate materials control the structure of water at the interface and in the interlayer space of these phases, as well as the effective diffusion rates of surface-sorbed species, their residence times at specific surface sites, and their translational and librational dynamics. At some surfaces, H_2O molecules can donate hydrogen bonds to the surface and can also accept H-bonds from the surface OH groups, thus developing a strong H-bonding network across the interface. However, at many interfaces the formation of such an interfacial H-bonding network is prevented by the unfavorable surface charge distribution. MD simulations complement the results of spectroscopic and other experimental measurements and allow us to merge greatly different time and length scales in understanding and predicting the properties of these materials.